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Fast integration of PDEs combining POD and Galerkin projection based on a limited set of mesh points

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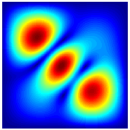
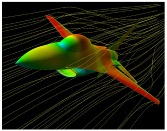
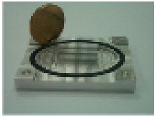
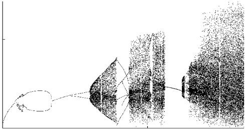
Motivation

- ★ Flow simulations are required for various **tasks** (design, control, stability analysis, ...) in many **fields** (engineering, physics, biology, ...)
- ★ **Huge computational resources** are often involved ($Re \gg 1$)

- ★ **Reducing the computational resources** required by standard numerical solvers is crucial in industrial applications

- ♣ **Numerical complexity** (number of grid points or cells) is often *much larger* than **physical complexity** (spatio-temporal features)

Scope & goal

Reduced order modeling (ROM) work is needed to (personal view):

- **Finding new ROM paradigms** (basic research) keeping in mind their computational efficiency.
- Combining 'known' ROM ingredients to **implementing flexible, robust ROMs** (applied research). Huge acceleration factors (say, 100-1000 or more) are required for industrial applications (Lucia *et al.*, Prog. Aerosp. Sci. 40, 2004)

This talk falls into the second class

GOAL. A robust, adaptive, 'customized spectral' method to decrease the cost to simulate time dependent dynamics of *dissipative* systems

For details, see Rapun, Terragni, V., Int. J. Numer. Meth. Engng. 2014 (in press; published online at http://onlinelibrary.wiley.com/)

Outline

Outline

1. Background
2. POD ‘on the fly’+additional ingredients
3. Numerical Results
4. Final Remarks

Preprocessed reduced order models

Given a **dissipative system**, the state vector $\boldsymbol{q}$ is assumed to belong to the linear subspace spanned by a few modes

$$\boldsymbol{q}(\boldsymbol{x},t) \simeq \boldsymbol{q}^n_{\mathrm{GS}} = \sum_{j=1}^{n} A_j(t)\boldsymbol{Q}_j(\boldsymbol{x})$$

- The **modes** $\boldsymbol{Q}_j$ can be computed using various methods from a representative set of snapshots calculated in a pre-process.
- The (unknown) **amplitudes** A_j calculated from a low-dimensional system obtained by projecting the governing equations onto the modes

Strengths/drawbacks:

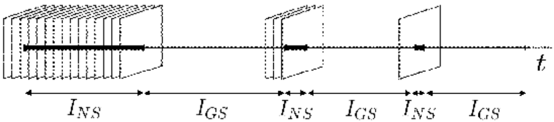
- ✓ Fast online operation (good for many-query scenarios)
- ✓ Expensive preprocess (sampling needed)
- ✓ Good to simulate attractors, not transients
- ✓ The mode truncation instability must be dealt with

Outline

POD ON THE FLY (MAIN IDEA)

This method combines on the fly, in interspersed time intervals:

- ★ A numerical solver (NS) used to POD-calculate when needed some snapshots that give the initial and updated POD manifolds
- ★ A Galerkin systems (GS) based on the n_1 most energetic POD modes. Projection based on limited ($\sim 3n_1$), equispaced set of points



Advantages/drawbacks:

- ✓ No preprocess needed; slower online operation than preprocessed ROMs.
- ✓ Good when the system is to be simulated just once (or few times)
- ✓ May be used to speed-up the pre-process in preprocessed ROMs
- ✓ Good for simulating complex transients, not only attractors
- ✓ Truncation instability bypassed

POD on the fly (need for updating detected)

The need to update the POD modes detected when either:

★ **Truncation error** not small enough

$$E_n^{n_1} = \frac{||\boldsymbol{q}_{\mathrm{GS}}^{n_1} - \boldsymbol{q}_{\mathrm{GS}}^{n}||}{||\boldsymbol{q}_{\mathrm{GS}}^{n_1}||} \equiv \frac{\sqrt{\sum_{j=n+1}^{n_1} |A_j|^2}}{\sqrt{\sum_{j=1}^{n_1} |A_j|^2}} < \varepsilon$$

★ The GS is being destabilized by the neglected modes (**mode truncation instability**). Can be monitored:

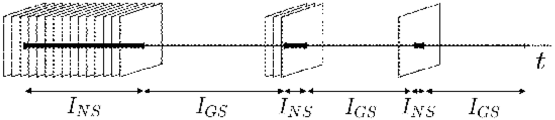
- Comparing with a second instrumental GS retaining more modes (old version, in, e.g., Rapún & V., JCP 229, 2010 ; Terragni *et al.*, SIAM J. Sci. Comput. 33, 2011); essentially doubles the GS CPU time.
- Using a normalized residual of the GS (this talk)

$$E_{\mathrm{res}}^{n_1} < \frac{\varepsilon}{k}$$

Residuals already used in reduced order modeling for different purposes in, e.g., Bergmann *et al.*, JCP 228, 2009 ; Grepl & Patera, M2AN 39, 2005

POD on the fly (updating strategy)

POD basis completely constructed at the outset, then only **updated on demand** to preserve the GS accuracy

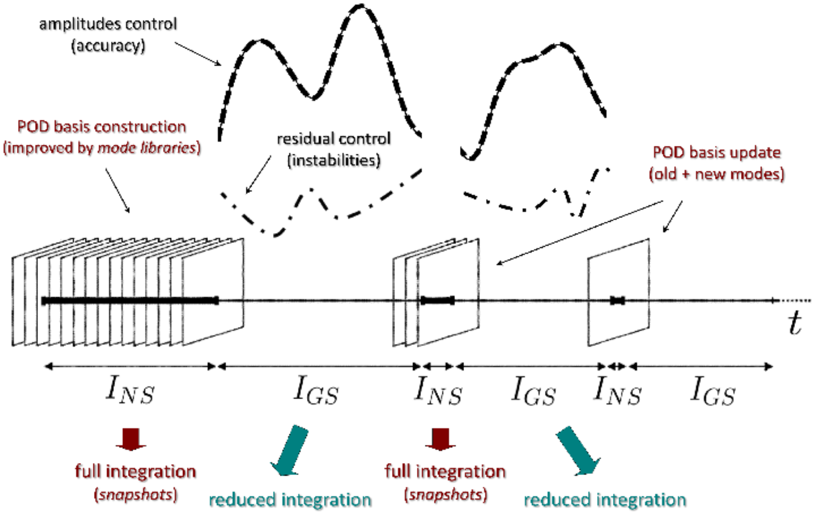


The POD subspace is updated ('rotated') by applying POD to the set of vectors $\underbrace{\hat{\nu}_1 \hat{\boldsymbol{Q}}_1, \ldots, \hat{\nu}_{N_1} \hat{\boldsymbol{Q}}_{N_1}}_{\text{old modes}}, \underbrace{\nu_1 \boldsymbol{Q}_1, \ldots, \nu_{N_2} \boldsymbol{Q}_{N_2}}_{\text{new modes}}$, where

$$\hat{\nu}_j = \min\left\{ \frac{\hat{\sigma}_j}{\sqrt{\sum_{k=1}^{N_1} (\hat{\sigma}_k)^2}}, \frac{\langle |A_j| \rangle}{\sqrt{\sum_{k=1}^{N_1} \langle |A_k| \rangle^2}} \right\}, \quad \nu_j = \frac{\sigma_j}{\sqrt{\sum_{k=1}^{N_2} (\sigma_k)^2}}$$

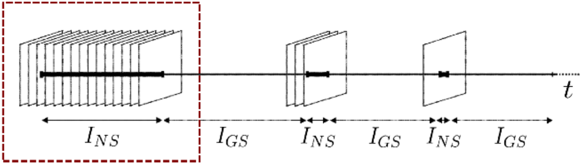
which makes **the POD modes dependent on the *local* dynamics**

POD ON THE FLY (SUMMARY)



POD on the fly (new ingredient)

The most computationally expensive step is the POD basis construction



How can the number of number of required initial snapshots be drastically reduced?

Mode libraries

- ★ The POD subspace depends only *weakly* on the problem parameters, in particular, on time
- ★ POD modes computed for some parameter values may be good for other values or even for other equations/discretizations (impressive examples in Terragni & V., Physica D 241, 2012)
- ★ The number of initial snapshots can be decreased by using a **mode library** as 'old modes set' at the outset, letting the updating strategy to adapt these modes as time proceeds

Useful *mode libraries* may come from:

- ✓ Applying POD to a set of generic functions (e.g., orthogonal polyn.)
- ✓ The final POD basis of a previous simulation with the reduced model (with any parameter values)
- ✓ Mixing up (via POD) different sets of modes of the above types

Outline

The 1D complex Ginzburg-Landau equation [1]

CGLE with homogeneous Dirichlet boundary conditions in 1D

$$\partial_t q = (1 + \mathrm{i}\alpha)\partial^2_{xx} q + \mu q - (1 + \mathrm{i}\beta)|q|^2 q \quad \text{with} \quad q = 0 \ \text{at} \ x = 0, 1,$$

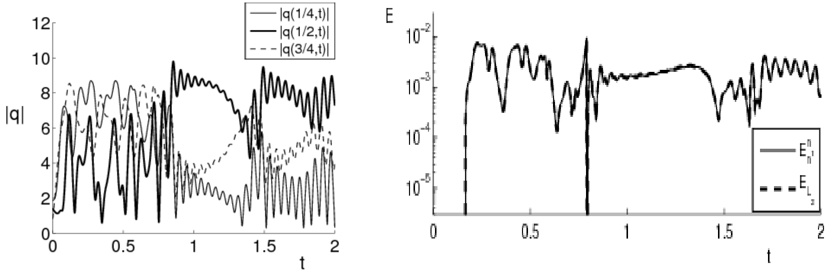
where q is complex and (α, μ, β) are real parameters

- ★ Paradigm describing a variety of phenomena (near Hopf bifurcations in extended systems)
- ★ Modulational instability if $\alpha\beta < -1$ and $\mu \gg 1$ (*complex* dynamics)
- ★ Very fast timescale $t \sim 1/\mu$ if $\mu \gg 1$
- ★ NS based on finite differences
- ★ The **speedup** will be measured as $\dfrac{\text{CPU time (NS)}}{\text{CPU time (reduced model)}}$

[1] Aranson & Kramer, Rev. Mod. Phys. 74 (2002)

1D CGLE: MODERATE COMPLEXITY

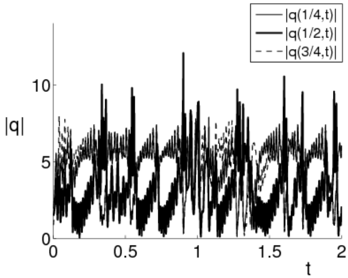
- ✓ $(\alpha, \mu, \beta) = (1, 80, -2.5)$, required accuracy $\varepsilon = 10^{-2}$
- ✓ errors set to zero where snapshots are NS-computed
- ✓ comparison restricted to a suitable timescale (needed for unstable dynamics)

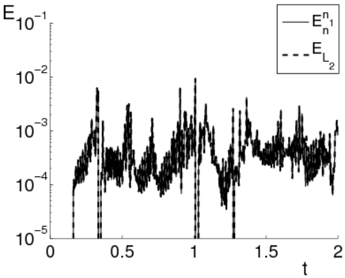


- ★ $E_n^{n_1}$ is a good estimate of the actual relative RMS error E_{L_2} (*vs.* NS)
- ★ $(n, n_1) = (9, 14)/(10, 15)$ in the first/second I_{GS} interval
- ★ **speedup ≈ 7.06**

1D CGLE: FULL CHAOS

✓ $(\alpha, \mu, \beta) = (1, 125, -20)$, required accuracy $\varepsilon = 10^{-2}$





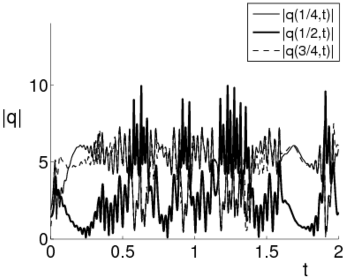
★ $E^{n_1}_{\text{res}}$ helps to prevent truncation instabilities (due to drastic transitions)

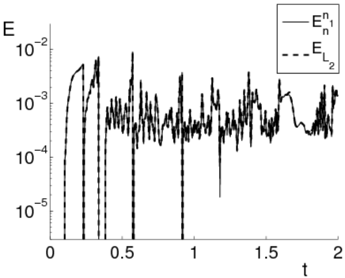
★ $(n, n_1) \sim (23, 33)$ in all I_{GS} intervals

★ **speedup ≈ 3.63** (higher complexity)

1D CGLE: INTERMITTENCY

✓ $(\alpha, \mu, \beta) = (0.75, 100, -13)$, required accuracy $\varepsilon = 10^{-2}$



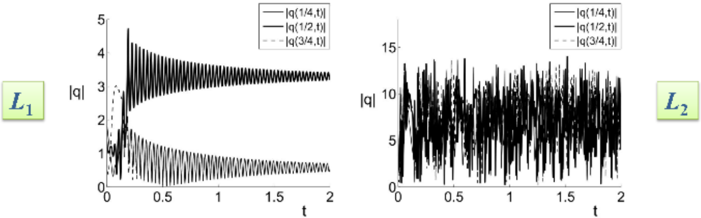


★ the POD subspace needs to be updated 4 times for an accurate description

★ **speedup ≈ 3.70**

Three mode libraries for the 1D CGLE

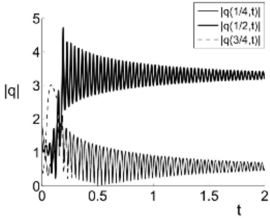
★ **Two particular mode libraries** (one simple, one complex) resulting from particular runs of the method

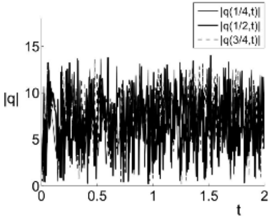


★ **One generic library** L_F: rescaled Fourier modes, $\frac{1}{n}\sin n\pi x$

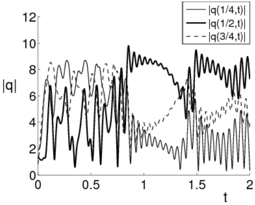
1D CGLE & MODE LIBRARIES: MODERATE COMPLEXITY

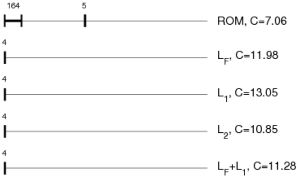
L_1





L_2

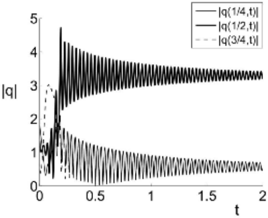


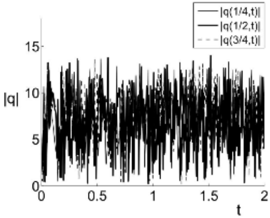


- ★ All libraries improve the performance of the reduced model (the number of snapshots is decreased, the speedup C is enhanced)
- ★ Modes from complex dynamics are better (even for fairly different parameters)
- ★ Mixing libraries allows to cover a significant part of the phase space

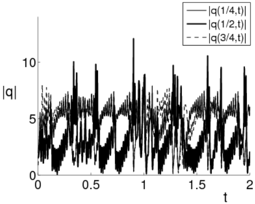
1D CGLE & mode libraries: chaos

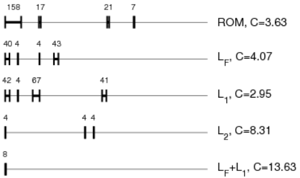
L_1





L_2





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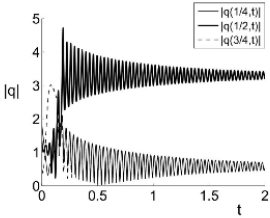
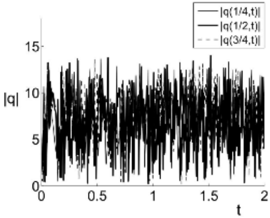
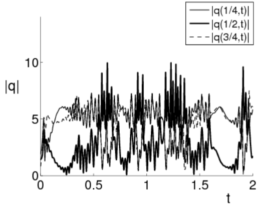
1D CGLE & MODE LIBRARIES: INTERMITTENCY

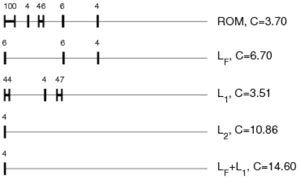
L_1





L_2





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The 2D complex Ginzburg-Landau equation [2]

The 2D CGLE with homogeneous Dirichlet boundary conditions is

$$\partial_t q = (1+\mathrm{i}\alpha)\triangle q + \mu q - (1+\mathrm{i}\beta)|q|^2 q \quad \text{with } \; q = 0 \; \text{ at boundaries of unit square}$$

where q is complex and (α, μ, β) are real parameters.

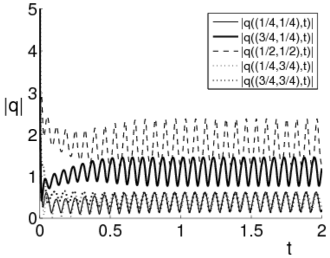
- ★ NS based on finite differences (uniform mesh with 250×250 points)
- ★ **Reduced model**: 16×16 grid points, required accuracy $\varepsilon = 10^{-2}$
- ★ Mode libraries also considered for improvement

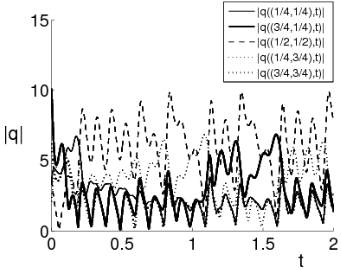
[2] Aranson & Kramer, Rev. Mod. Phys. 74 (2002)

2D CGLE: TWO EXAMPLES

Left

- ✓ periodic dynamics: $(\alpha, \mu, \beta) = (-1, 50, 30)$; required accuracy: $\varepsilon = 10^{-2}$
- ✓ **speedup $\approx$ 9.13**





Right

- ✓ complex dynamics: $(\alpha, \mu, \beta) = (1, 80, -2.5)$; required accuracy: $\varepsilon = 10^{-2}$
- ✓ **speedup $\approx$ 2.61**

Three mode libraries

Mode libraries

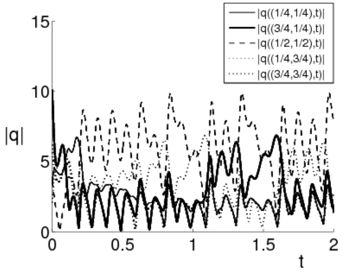
- ★ A first generic library ℓ_{F1} contains the 83 weighted Fourier modes

$$\frac{1}{\sqrt{m^2+n^2}} \sin m\pi x \sin n\pi y,$$

  such that $\sqrt{m^2+n^2} \leq 11$
- ★ A second generic library ℓ_{F2} contains the 117 weighted Fourier modes such that $\sqrt{m^2+n^2} \leq 13$
- ★ A particular mode library ℓ_1 contains the 40 most energetic POD modes resulting from the application of the method for the same parameter values as the simplest particular library considered in 1D

These libraries are simpler than those considered in 1D

2D CGLE: MODE LIBRARIES & SPEEDUP

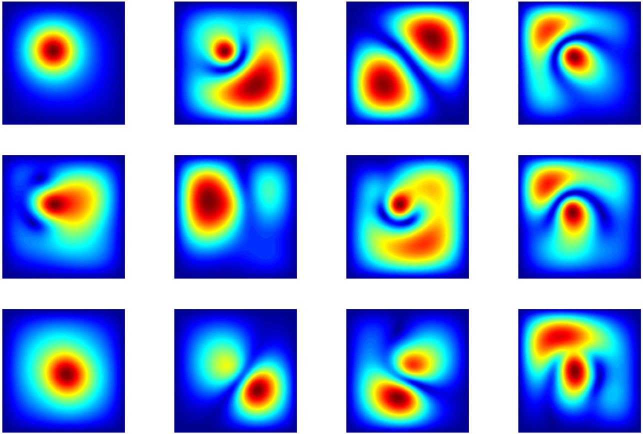


	ROM	ℓ_{F1}	ℓ_{F2}	ℓ_1	$\ell_{F1}+\ell_1$	$\ell_{F2}+\ell_1$
C_{theor}	2.66	31.74	100	3.13	40.81	500
C	2.61	26.91	90.96	3.04	35.42	357.60

TABLE: theoretical & CPU speedup when applying the reduced order model alone (ROM) and with the indicated mode libraries

2D CGLE: MODES ADAPTIVITY

The modes change with time & *adapt* to the actual dynamics.



First 4 modes in the library $\ell_{F1} + \ell_1$ (*row* 1), in the first I_{GS} interval (*row* 2), and in the last I_{GS} interval (*row* 3)

Outline

Summarizing

1. A robust & flexible method based on POD on the fly and mode libraries was presented
2. The low dimensional modeling combines a GS & a standard NS for a fast simulation of unsteady – *transient* – dynamics in some dissipative systems
   - ✓ POD subspace updated 'on the fly' to preserve accuracy
   - ✓ mode truncation instability bypassed using an appropriate *residual estimate*
   - ✓ performance enhanced using *mode libraries*
3. Application to the CGLE was illustrated in 1 & 2 spatial dimensions, showing a remarkable speedup (up to 15 & 360, respectively) using not-optimized software/libraries selection
4. Similar reduced models were also constructed for other applications
   - ★ Laminar flows in a driven cavity (Terragni *et al.*, SIAM JSC 33, 2011)
   - ★ Complex bifurcations diagrams (Terragni & V., SIADS 13, 2014)
5. Combining these ideas with *multiscale descriptions* would hopefully allow to handle more complex problems